MEASUREMENT OF LONGITUDINAL DISPERSION IN STREAMS AND ITS APPLICATION USING A WATER QUALITY MODEL

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ABSTRACT

QUAL2E is one of the most widely used water quality model for watershed and stream management. It is capable of estimating the wasteload allocation or total maximum daily load (TMDL) for a given stream or river. The predictive equations used in QUAL2E were developed in United States and England; therefore, the applicability of QUAL2E in Malaysia with different climatological and geological conditions needs to be studied. In modeling, the accuracy of simulation is highly dependent upon the accuracy of empirical coefficients used, such as longitudinal dispersion. In this study, a water quality model upstream of Tebrau River was calibrated. The accuracy of the use of default dispersion constant, K (dimensionless), in water quality model (QUAL2E), for predicting the longitudinal dispersion effect of stream was examined. Longitudinal dispersion coefficients also calculated from predictive equations. Finally, an error analysis was conducted to compare the standard error (SE) of model outputs resulted from different longitudinal dispersion coefficients and evaluated which method gave the best result.

INTRODUCTION

Mixing mechanism of water in stream is basic stream flow characteristic that helps to estimate the rate of movement and dilution of pollutants that may be introduced into streams (Jabson, 1996). Spreading pattern of pollution will greatly affect the water quality along the whole river. Advancement in computer today provides a numerical mean to predict the effect of mixing on stream water quality. Initially, water quality model was designed as a problem-solving tool. For example, calculate the waste load allocation for a stream and use to overcome a pollution problem. Besides from these functions, a water quality model can provide a quantitative framework, which integrates different physical, chemical and biological information that constitute to the complex environment.

All water quality models available need to be calibrated and validated for a particular stream before it can be used confidently. Therefore, determinations of accurate input information and kinetics such as longitudinal dispersion are vital in water quality modeling.

In Malaysia the increasing growth of population and industry within the watershed will make the water quality standard more difficult to comply. Water quality model, such as QUAL2E is needed for river management to control the discharge of domestic and industrial wastewater into river. However, QUAL2E was developed in US. Before the model could be used, the users have to determine weather it is applicable in Malaysia condition. Different geological, climatological conditions found in Malaysia have will affect the transport mechanism of streams and eventually result water quality changes.

Propose of this study is to examine the accuracy of the use of default dispersion constant, K (dimensionless), in water quality model (QUAL2E), for predicting the longitudinal dispersion effect of stream. A water quality model upstream of Tebrau River was calibrated. Meanwhile, longitudinal dispersion coefficient can also be obtained from several predictive equations. Model simulations using dispersion constants calculated from different predictive equations were studied. Finally, error analyses were conducted to compare the results from different dispersion coefficients.

THEORIES AND MATERIALS

Longitudinal Dispersion in Streams

Mixing mechanism of effluent discharged into streams can be categorized into 3 stages. The rate of mixing in the initial stage is dominated by the momentum and buoyancy of the effluent itself. When the effects of initial momentum and buoyancy are diluted after the first stage, the turbulence occurred naturally in the stream will mix the waste across the river during the second stage. In the last stage, where the effluent has been well-mixed across the river, longitudinal mixing will take place to eliminate the concentration difference along the stream (Fisher et al. 1979).

Longitudinal dispersion is a combined effect of turbulent mixing and shear flow effect, however, the former is only minor important. The motion of each water molecule in a uniform stream is a stationary random function. However, in the stream the primary mechanism for spreading out is the time-steady cross-sectional variation of velocity. In contrast, in turbulent diffusion, the only mechanism is random temporal velocity variations (random steps forward or backward). The spatial velocity variations in a stream are far more effective at spreading out than are the temporal variations. Since both mechanisms are so different, the terms " dispersion" for spreading out due to spatial velocity differences, and "diffusion" for spreading by random temporal fluctuations should not be interchanged (Fisher, 1968).

Previous Studies on Longitudinal Dispersion

The one-dimensional dispersion model, as originally formulated by Taylor (1954), state that a dispersing cloud of tracer may be described by a bulk diffusion equation

$$\frac{\partial c}{\partial t}+U\frac{\partial c}{\partial x}=D\frac{\partial^2 c}{\partial x^2} \tag{1}$$

Where c is the concentration at a distance x and time t, U is the mean flow velocity, and D the longitudinal dispersion coefficient. Equation 1 states that the entire cloud is advected downstream at the mean-flow velocity while spreading out according to the classical equation for molecular or heat diffusion.

In open channel flow, Elder (1959) assumed a logarithmic vertical-velocity distribution to give the well know equation

$$D_L = 5.93HU^* \tag{2}$$

Where U^* is the bed shear-stress velocity, H the depth of flow. However, it had been found that Elder's equation does not accurately describe longitudinal dispersion in natural streams and channels. Guymer and West (1992) confirmed the importance of both vertical and transverse shear components of the longitudinal dispersion coefficient, according to the measurements of velocity and salinity distributions on a cross-section in the Conwy estuary in UK. Studies undertaken using many measured data sets for natural rivers have shown that the value of D_L/HU^* may vary from 8.6 to 7500, with values generally being much greater than Elder's equation constant of 5.93.

In applying Taylor's assumptions to the mass-conservation equation for turbulent flow, and assuming that transverse or lateral variations are more important, Fischer (1967) presented a new equation for D_L. This equation was based on integrating the time-independent portion of the resultant conservation of mass equation over the depth and including the boundary condition of no mass flux across the bed and water surface. The resulting equation was in the form of

$$D_L = -\frac{1}{A}\int_0^W U'(y)H(y)\int_0^y \frac{1}{\varepsilon_y H(y)}\int_o^y U'(y)H(y)dydydy \qquad (3)$$

Where U' is the spatial deviation of the velocity from the cross-sectional mean velocity, as a function of distance in the y direction, W is the channel width, y direction and ε_y the lateral turbulent mixing coefficient in y direction, which has been found, by experiment, to be typically in the region of $0.23HU^*$-$0.7HU^*$.

In estimating D_L for practical engineering studies, it has become preferable to use equations which are based on the hydraulic and geometric parameters, and which can be readily obtained from numerical models, to represent D_L. McQuivey and Keefer (1974) presented such an equation, based on combining the linear one-dimensional flow and dispersion equations, to give

$$D_L = 0.058\frac{Q}{SW}, \qquad for \;\; F_n \langle 0.5 \qquad (4)$$

Where Q is the discharge at steady base flow, S the slope of energy line, and F_n the Froude number.

Fischer developed a simple method to predict the longitudinal dispersing coefficient, which is a simplified non-integral from Equation 3, giving

$$D_L = \frac{0.07U'^2\, l^2}{\varepsilon_y} \qquad (5)$$

Where l is the distance from the point of maximum velocity to the most distant bank. From laboratory experiments, Fischer found that U'^2/U^2 varied typically from 0.17 to 0.25, with a mean value of 0.2, and l was typically equal to $0.7W$. By substituting these two values in eqn 1 and setting $\varepsilon_y = 0.6\,HU^*$, he concluded that D_L could be obtained from

$$D_L = \frac{0.011U^2W^2}{HU^*} \qquad (6)$$

Seo and Cheong (1998) have published new equations for predicting the longitudinal dispersion coefficient, derived from dimensional analysis and a regression analysis for the non-step Huber method using 59 data sets, and measured data in 26 rivers in the USA. They used 35 of these measured data sets to establish their equation and then verified it against other data sets. Their equation can be written as

$$\frac{D_L}{HU^*} = 5.915\left(\frac{W}{H}\right)^{0.620}\left(\frac{U}{U^*}\right)^{1.428} \qquad (7)$$

Water Quality Model – QUAL2E

The present QUAL2E software package was an effort of U.S. Environmental Protection Agency (USEPA) for wasteload allocations, discharge-permit allocations and other pollution evaluations (Maketab, 2001). It is presently the most widely used computer model for simulating stream-water quality. QUAL2E has its root in the QUAL-I model developed in 1970. The model was upgraded several times to become the present version (Brown and Barnwell, 1987) of "Enhanced QUAL-II Model" or "QUAL2E" for short.

QUAL2E can simulate up to 15 water quality constituents. The model is applicable to simulate dendritic stream that are well mix. It assumes that the main transport mechanisms, advection and dispersion, are significant only along the main direction of flow (longitudinal axis of the stream). It allows for multiple waste discharges, withdrawals tributary flows and incremental inflow and outflow. It also has the capability to compute required dilution flows for flow augmentation to meet the pre-specified dissolved oxygen level. (Chapra, 1997)

Hydraulically, QUAL2E is limited to the simulation of time periods during which both the stream flow in river basins and input waste loads are essentially constant. QUAL2E can operate either as a steady state or as a dynamic model. When operated at steady state, it can be used to study the impact of waste load on stream water quality and also to identify the magnitude and quality characteristic of non-point source waste loads. By operate dynamically, the effects of diurnal variation in meteorological data on water quality and diurnal dissolved oxygen variations due to algae growth and respiration can be observed.

QUAL2E subdivides the stream system in to reaches, which are stretches of stream that have uniform hydraulic characteristics. Each reach is then divided into computational elements of equal length. Reaction rate coefficients, initial conditions and incremental flow data are constant for all computational elements within a reach. Thus, the stream can be conceptualized as a string of completely mixed reactors (computational elements) that are linked sequentially to one anther via the mechanisms of transport and dispersion.

The one-dimensional mass transport equation of QUAL2E includes the effect of advection, dispersion, dilution, constituent reactions and interactions, and sources and sinks. This balance can be generally written as Equation 1

$$\underbrace{V\frac{\partial c}{\partial t}}_{\text{Accumulation}} = \underbrace{\underbrace{\frac{\partial\left(A_c D_L \frac{\partial c}{\partial x}\right)}{\partial x}dx}_{\text{Dispersion}} - \underbrace{\frac{\partial(A_c U c)}{\partial x}dx}_{\text{Advection}}}_{\text{Transport}} + \underbrace{V\frac{dc}{dt}}_{\text{Kinetics}} + \underbrace{s}_{\text{External sources/sinks}} \qquad (8)$$

Where V = volume, c = constituent concentration, A_c = element cross-sectional area, D_L = longitudinal dispersion coefficient, x = distance, U = average velocity, s = external sources or sinks of the constituent.

Longitudinal Dispersion Prediction in QUAL2E

QUAL2E model uses Elder's equation (Equation 2) to predict the longitudinal dispersion effect in stream, which assumed that only the vertical velocity gradient was important in stream flow. Equation 2 can be written in terms of the Manning Equation and other variables characteristic of stream channels. For example

$$U^{*} = C\sqrt{RS_e} \tag{9}$$

$$C = \frac{R^{1/6}}{n} \tag{10}$$

$$S_e = \left(\frac{\overline{U}n}{1.486R^{2/3}}\right)^2 \tag{11}$$

Where C = Chezy's coefficient, R = the hydraulic radius, S_e = the slope of the energy, n = Manning's roughness coefficient. Substitute equation 9, 10 and11 into equation 2 yields the expression

$$D_L = 3.11\ KnUH^{5/6} \tag{12}$$

Where D_L = longitudinal dispersion coefficient (m^2/s), n = channel's roughness coefficient (dimensionless), U = mean velocity (m/s), H = mean depth (m), K = dispersion parameter (dimensionless), defined as

$$K = \frac{D_L}{HU^{*}} \tag{13}$$

Where U^{*} = shear velocity (m/s). These two equations are representing a circular reasoning.

METHODOLOGY

Study Area – Upstream of Tebrau Watershed

The Sg Tebrau is located south of the state of Johor. It flows through the administrative area of Majlis Bandaraya Johor Bahru (MBJB), Majlis Perbandaran Johor banhru Tengah (MPJBT), Majlis Daerah Kulai (MDK) and a small part of Majlis Daerah Kota Tinggi (MDKT). Land use upstream of Tebrau River is dominated by palm oil and rubber plantations. Downstream of river is mainly covered by build-up areas, occupied by residential, municipal and industrial areas. Sg. Tebrau is approximately 32.5 km in length and its catchment area is approximately 257.4 km^2. Sg Tebrau is divided into 2 zones by the presence of the Public Utilities Board (PUB) of Singapore barrage built in the late 1940's. The rainfall pattern in this region is strongly influenced by two major air streams: the northeast monsoon, which blows from November/December to March and the southwest monsoon between May and September/October. The annual rainfall ranges from 1860 to 2763 mm, with an average of 2279 mm. (IEWRM, 2002)

The study of longitudinal dispersion coefficient in Sg. Tebrau is confined to only upstream freshwater zone, which include area from Chai Nyet Chok Oil Palm Plantation, east of Senai Air Port, to Kg Maju Jaya.

Table 1: Gauging and Water Quality Monitoring Station.

Station No	River	Station	Location	
1	Tebrau	Senai Industrial Park	N 01°38.302'	E 103°40.645'
2	Tebrau	Solid Mesh	N 01°37.100'	E 103°41.129'
3	Tebrau	Jalan Kampung Tawakal	N 01°35.439'	E 103°42.828'
4	Tebrau	Kg Maju Jaya	N 01°34.889'	E 103°43.050'
5	Tebrau	Landscape Kg Maju Jaya	N 01°34.445'	E 103°43.251'

Five water gauging and water quality monitoring stations are suggested along the study area (Table 1). Hydraulic and water quality data required for calibration and validation of QUAL2E model are measured.

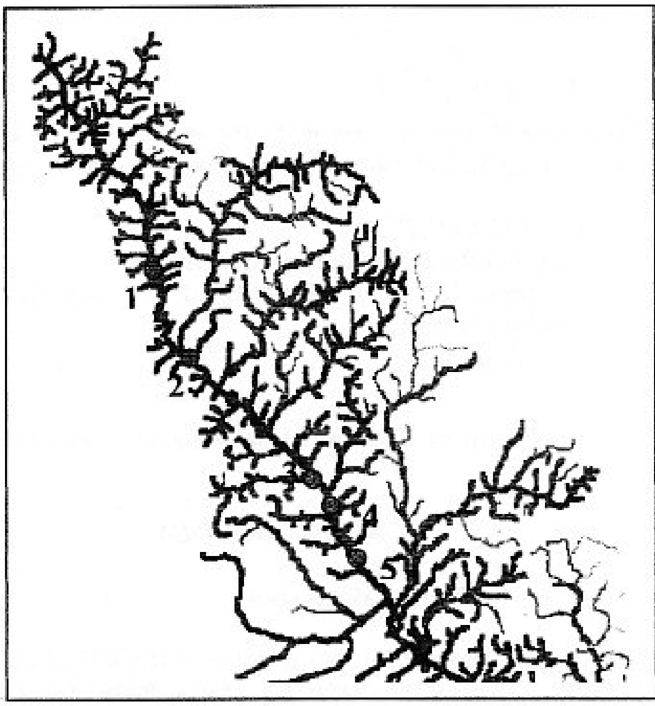

Figure 1: Upstream of Tebrau River Network and Selected Monitoring and Gauging Station.

Data Collections

Hydraulic data including velocity, width, and depth changes across the river, and flowrate are measured in each water gauging and water quality monitoring station for 8 different days. Water quality parameter such as BOD, COD, DO, temperature, salinity, conductivity, ammoniacal nitrogen, nitrite and nitrate and phosphate were examining from samples taken at each stations. These hydraulic and water quality data became the input data for the QUAL2E simulation.

Model Calibration

Reliability of a water quality model needs to be determined by calibration and validation process before the model is being used. Calibration process is to calibrate or "tune" the model to fit a data set. This consists of varying the model parameters to obtain an optimal agreement between the model calculations and the data set. There are several types of information that must be fed into the model. These include the forcing functions and physical parameters (boundary conditions and loads, initial conditions, physics) and calibration parameter (kinetics). Figure 2 schematically shows the systematic way to complete the calibration process (Chapra, 1997).

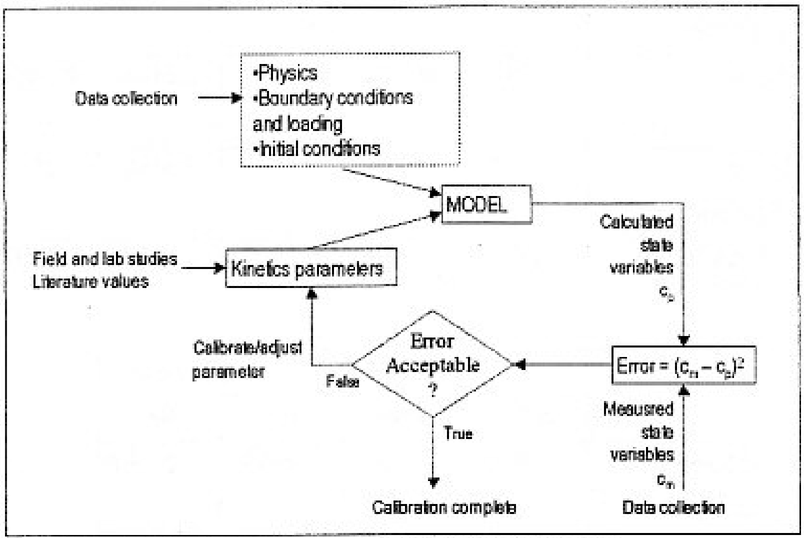

Figure 2: Schematic Diagram of the Model Calibration Process

Model calibration process was done by tuning the model to fit data on 25 September 2002. In calibration process, dispersion constants were set as default, 60. Later, longitudinal dispersion coefficients calculated from different predictive equations were then replacing the default value. Simulated water quality results from different dispersion values were compared to the measured data from 5 sampling and gauging stations. Error analyses were conducted to evaluate the SSE (sum of squares of errors), MSE (mean of squares of errors) and SE (standard error) of the output results.

RESULTS

Simulation results from various predictive equations were diverse for different water quality parameters. Fisher equation, Seo and Cheong equation and default value in QUAL2E showed the similar results (same SE) for DO and performed better than the McQuivey and Keefer equation, which gave relatively higher SE. For BOD, the trend changed with McQuivey and Keefer equation gave the best result (lowest SE), followed by the Seo and Cheong equation as well as default value, and lastly Fisher equation. However, for COD, sequence in ascending order (lowest to highest SE) was default value, Fisher equation and Seo and Cheong equation, McQuivey and Keefer equation. Meanwhile, the summation of the SE for these 3 water quality parameters during calibration process indicated that, the ascending SE sequence was McQuivey and Keefer equation, default value, Seo and Cheong equation and Fisher equation (Table 2).

Table 2: Error Analysis of Calibration Results for DO, BOD and COD, Upstream of Tebrau River.

	DO			BOD		
	SSE	MSE	SE	SSE	MSE	SE
McQuivey and Keefer Predictive Equation	0.1766	0.0353	0.1879	2.4883	0.4977	0.7055
Fisher Predictive Equation	0.1743	0.0349	0.1867	2.5194	0.5039	0.7099
Seo and Cheong Predictive Equation	0.1743	0.0349	0.1867	2.5188	0.5038	0.7098
Default in QUAL2E, 60	0.1743	0.0349	0.1867	2.5188	0.5038	0.7098

(continued)

	COD			Total
	SSE	MSE	SE	SE
McQuivey and Keefer Predictive Equation	17.9638	3.5928	1.8955	2.7888
Fisher Predictive Equation	17.9879	3.5976	1.8967	2.7933
Seo and Cheong Predictive Equation	17.9879	3.5976	1.8967	2.7932
Default in QUAL2E, 60	17.9478	3.5896	1.8946	2.7911

CONCLUSIONS

Longitudinal dispersion coefficient is proportional to the squares of the distance over which the shear flow profile extends (Fisher et al., 1979); the effect will become greater as the width of the river increases. The width range of the study area is between 5 meters to 10 meters, completed mixing is easily achieved in this area, thus, diluting the effect of longitudinal dispersion on stream water quality.

The wasteload from the point and non-point sources were difficult to estimate considering that even hydraulic and water quality data upstream of Tebrau River was limited. Underestimation of the wasteload would make the effect of mixing in stream difficult to be observed, it is because the pollution load would be regarded contributed by the incremental flows instead of pollution sources.

The calibration results shown above indicate that there is no one predictive equation is best for all water quality parameters along the whole river system. However, since only calibration process was carried out, further verification is needed in order to make a comprehensive conclusion.

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